LA-UR-88- 633

LA-UR--88-633

DE88 006445

TITLE **THE TURBULENT HEAT FLUX IN LOW MACH NUMBER FLOWS WITH LARGE DENSITY VARIATIONS**

AUTHOR(S) *Peter J. O'Rourke and Lance R. Collins*

SUBMITTED TO Workshop on Transport Processes in Dispersed Two-Phase Flows with Applications to Propulsion Systems. Held at NASA Marshall Space Flight Center, Huntsville, Alabama, February 25-26, 1988.

DISCLAIMER

Los Alamos National Laboratory
Los Alamos, New Mexico 87545

THE TURBULENT HEAT FLUX IN LOW MACH NUMBER FLOWS WITH LARGE DENSITY VARIATIONS

Peter J. O'Rourke and Lance R. Collins
Theoretical Division, Group T-3
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

I. INTRODUCTION: THE DIRECTED ENERGY FLUX

This paper is concerned with a physical effect of fundamental importance for the modeling of turbulence transport in flows with large density variations. The effect occurs because the interaction of pressure and density gradients gives rise to a turbulent heat flux, which we call a directed flux, that is not accounted for in turbulence models for constant density flows. To see how this flux arises, it is perhaps best to consider an example of Rayleigh-Taylor instability, as depicted in Fig. 1. A heavy, cold gas overlays a light, hot gas in a box with a gravitational acceleration in the negative z-direction. The induced hydrostatic pressure gradient accelerates the light gas into the heavy gas and causes the instability and mixing. The velocities averaged across a horizontal plane are in the z-direction, and because the heavy gases are falling, the mass-averaged velocities in the mixing region will be negative. Relative to a surface moving downward with the mass-averaged velocity, there will be a net upward flux of energy. This is because although the mass flux of light gas crossing the surface upward equals the mass flux of heavy gas crossing downward, the light gas, being hotter, carries with it more energy per unit mass.

This upward energy flux is the directed flux. In the example of Fig. 1, this energy flux is in the direction of the negative of the temperature gradient, just as given by the laminar Fourier heat conduction law. If after some time we were to turn the box over so that the light gas overlay the heavy gas, to the extent that the two gases had not already mixed on the molecular level, there would be an unmixing in which the light gas would separate from the heavy gas. In this

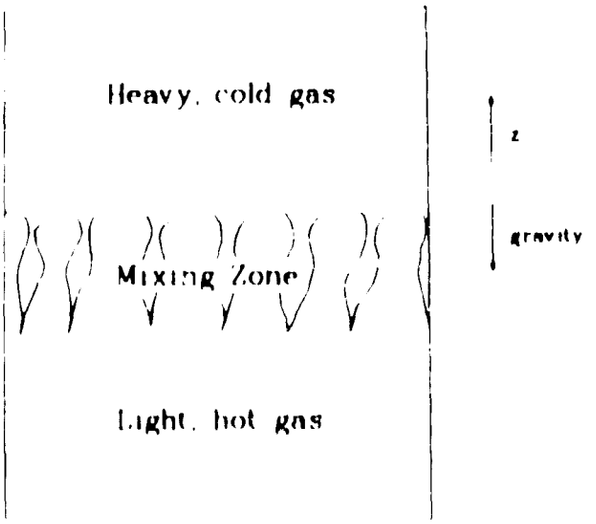

Fig. 1. Schematic depiction of Rayleigh-Taylor instability.

unmixing process, the directed heat flux would be upward, in the direction of the mean temperature gradient and opposite the direction given by the Fourier heat conduction law. This phenomenon has thus been called countergradient diffusion.[1] It cannot be predicted by turbulence models that use gradient transport, or a Fourier-like law, to describe turbulent heat transport. In our example, the turbulent heat flux ϕ^h is in the direction opposed to the pressure gradient, rather than the temperature gradient. We shall see that taking $\phi^h \sim -\nabla p$ is often more realistic for turbulent flows.

Between single-phase, two-density turbulent flows and two-phase flows there is an analogy that we will exploit in our turbulence modeling. This analogy will be used in helping to formulate the equations and in developing closure approximations for some of the terms. In two-phase flow modeling, which has received much attention within the last ten years[2,3] separate mass, momentum, and energy equations are kept for each phase, and these equations are coupled through functions that give the exchange rates of mass, momentum, and energy between the phases. Following Besnard, Harlow, and Rauenzahn,[4] we will use an alternative, analogous formulation. In place of two mass equations, we will keep an equation for the mean density and one for density fluctuations. In place of two momentum equations, we will keep a mean momentum equation and an equation for mean velocity differences associated with fluid elements of differing density. We use this second formulation because it allows for the possibility of modeling not just two-density flows, but the flows with a spectrum of densities that often occur in practical applications.

Two physical examples, one of two-phase flow and one of single-phase flow with density variations, serve to illustrate the analogy and another situation in which countergradient transport can arise. In both examples, pressure gradients are responsible for centrifuging lighter material inward toward the centers of rotating flows. In a two-phase bubbly flow, this effect has been observed in the vortices in the wake of an obstacle.[5] In single-phase flow, it is probably responsible for the experimental results of Wahiduzzaman and Ferguson.[6] The experimenters measured the radial temperature profiles in an axisymmetric swirling flow in a constant volume cylinder. The experimentally measured temperatures are plotted at four different times as the circles in Fig. 2. The lines are computed temperature profiles using the KIVA code[7] with a k-ε turbulence model[8] and gradient heat transport with a turbulent Prandtl number of 0.9. It can be seen that a hot region in the center of the cylinder persists much longer in the experiment than in the calculation, showing the large errors that can arise when a gradient heat transport approximation is used.

The phenomenon of countergradient transport in single-phase flows was recognized seven years ago in research on the structure of turbulent premixed flames.[1] In retrospect, it is easy to see how this phenomenon arises. Figure 3 depicts schematically a planar turbulent premixed flame with velocities shown in the frame of reference of the flame. Mass conservation and the fact that the combustion is nearly isobaric together imply that the hot product gas velocities will be larger than those in the reactants. Momentum conservation then implies that the pressure in the products will be lower than in the reactants. Since the directed heat flux is in the direction opposed to the pressure gradient, this heat flux will be from the colder to the hotter gases; that is, it will be countergradient transport.

Two approaches have been used for modeling turbulent premixed flames: a single-phase formulation and a two-phase formulation. In the single-phase formulation of Bray, Moss and Libby[1,9-11] (BML formulation), equations are kept for the mean product gas concentration, the mean momentum, the turbulent fluxes of these quantities, and for the dissipation rate of turbulent kinetic energy

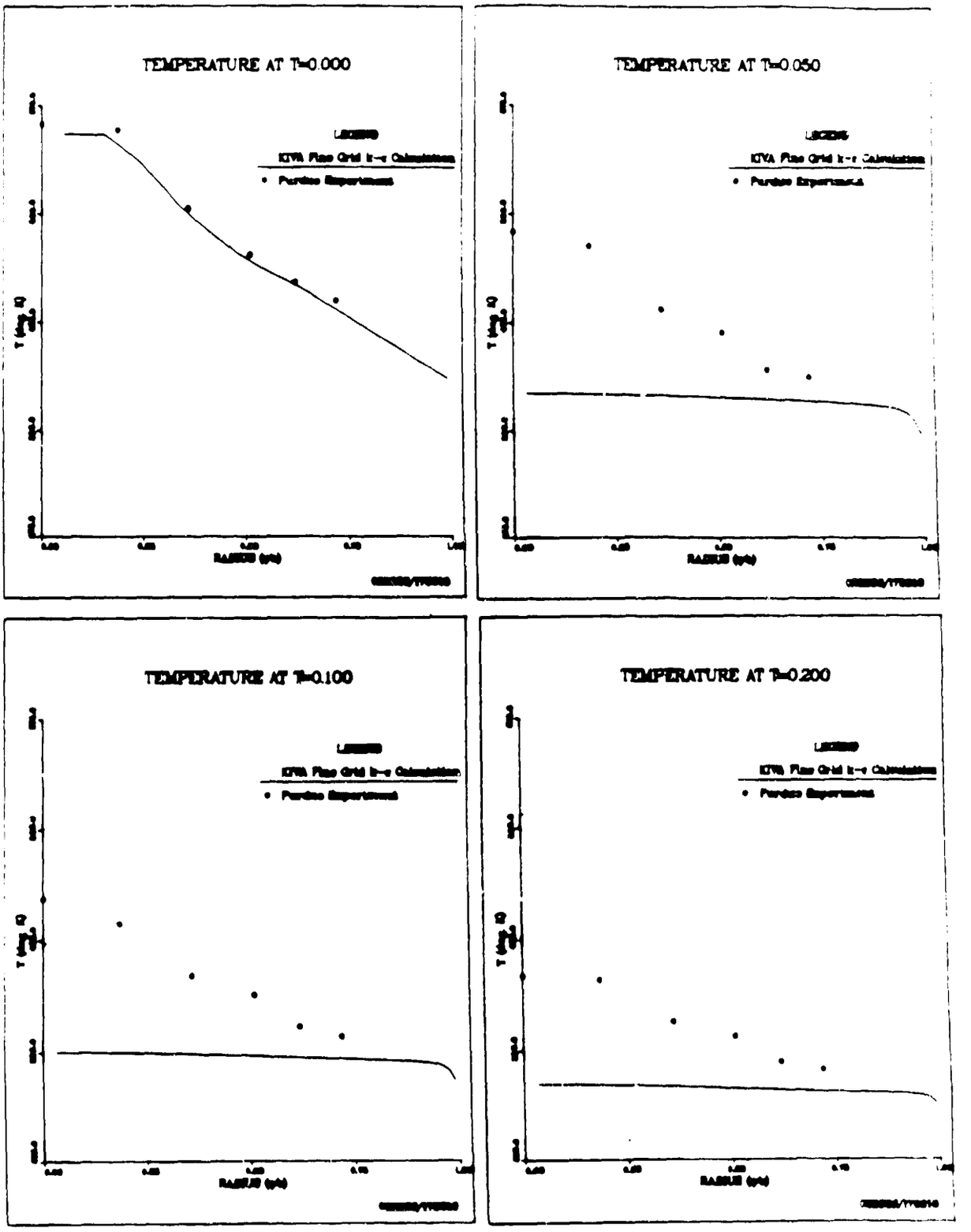

Fig. 2. Experimentally measured (Ref. 6) and computed (KIVA code) radial temperature profiles at four different times.

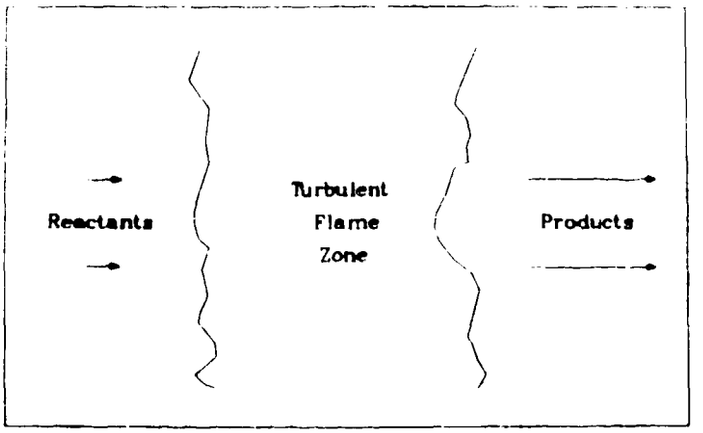

Fig. 3. Schematic depiction of a turbulent premixed flame.

Spalding[12] utilizes a two-phase formulation, retaining mass, momentum, and energy equations for each phase. Spalding[12] assumes that the major source of mixing is due to the difference between the mean velocity of the phases and thus ignores the turbulent kinetic energy within each phase. The BML formulation accounts for both sources to the turbulent kinetic energy. In principle, the equations of one formulation should be derivable in terms of those of the other, although to our knowledge such a derivation and comparison have not been made. In this paper some closure approximations are proposed, based on a derivation of the single-phase equations from two-phase equations. Only the BML formulation has been compared with experimental measurements of turbulent flames,[11] and satisfactory agreement was obtained.

In practical applications of turbulent combustion, other physical effects that cause mixing and unmixing are superimposed on the pressure drop across the flame. At Los Alamos, we have been involved for the past twelve years in the numerical modeling of combustion in internal combustion engines.[7,13-16] Figure 4 illustrates some of the complexities of the turbulence/chemistry interaction in an engine burning premixed charges. A turbulent premixed flame is propagating away from an ignitor located near the center of the cylinder head wall. Mach numbers are small, and thus the mean pressure is nearly uniform in space[17] and changing with time due to piston motion, combustion, and wall heat loss. Near the top of its motion, the piston, and the axial flow velocities in the combustion chamber, decelerate. This causes a small positive axial pressure gradient and induces Rayleigh-Taylor instability and mixing where the flame is propagating downward in the axial direction. This same pressure gradient will cause a differential axial acceleration of the hot products and cool reactants and promote Kelvin-Helmholtz instability where the flame is propagating radially. Swirl, a nearly symmetric rotational motion of the burning gases, is introduced by engine designers to promote mixing but will have two competing effects in the engine of Fig. 4. Swirl induced shears will enhance turbulence and mixing, but the radial pressure gradient caused by the swirl will, as in the experiments of Wahiduzzaman and Ferguson,[6] cause countergradient transport and suppress mixing. It is important to point out that among these various turbulence effects, only those associated with shear instability and mixing are accounted for in current engine models.

In predicting turbulence in internal combustion engines and other practical combustors, one cannot use two-phase models or single phase equations for two density flows. This is because within the reactants and products there will be

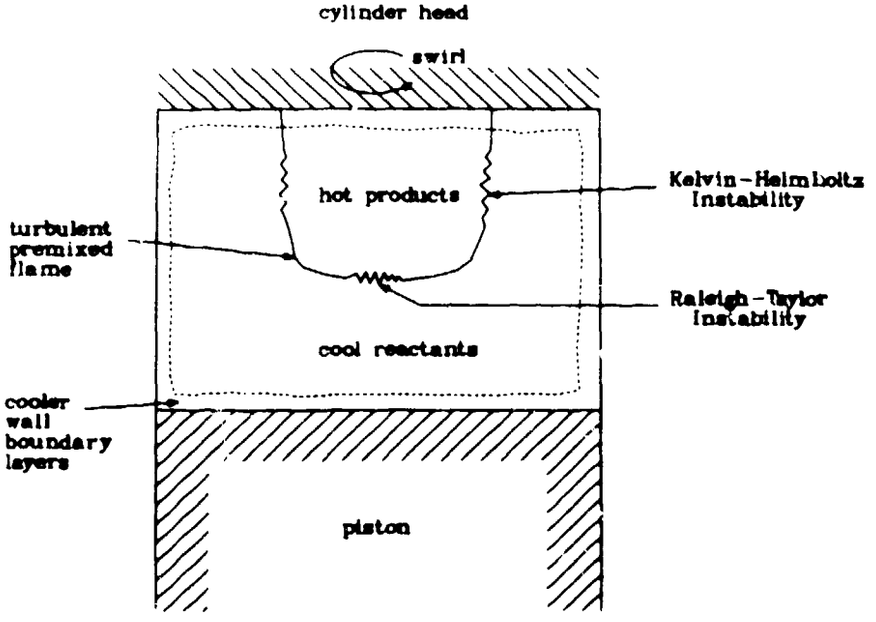

Fig. 4. The turbulence/chemistry interaction in an internal combustion engine.

distributions of density. In the engine of Fig. 4 density differences will arise due to wall heat transfer and due to entropy differences in the product gases of this confined burn.[18] In other combustors density distributions are caused by charge non-uniformity and spray vaporization.

In the next section we derive preliminary equations for a turbulent fluid with large density variations. Our aim is to develop a model that has three attributes:

(1) the model can predict mixing and unmixing due to shear instabilities and pressure-density gradient interactions;
(2) the model can account for a distribution of densities; and
(3) the model equations can be efficiently integrated in two and three dimensions.

The second attribute precludes use of two-phase flow equations, although investigation of the two-density limit will yield valuable information. The third attribute precludes use of the Reynolds stress equations, especially in three dimensions. It seems appropriate to seek a simple one- or two-equation extension of popular two-equation models for turbulent shear flows.

II. THE EQUATIONS

A. Overview

We first derive equations for the average density $\bar{\rho}$ and the Favre-averaged velocity $\tilde{u}$ and enthalpy $\tilde{h}$. Using the low Mach number assumption, we relate the turbulent heat flux ϕ^t to the difference between the average velocity $\bar{u}$ and the Favre-averaged velocity $\tilde{u}$. We denote this difference $\bar{u} - \tilde{u}$ by a, and the transport equation for a is derived and discussed. Closure approximations for terms in the a equation are postulated based on the analogy between two-phase flows and single-phase, two-density flows. A comparison between the single-phase and two-phase equations suggests that the fluctuating stress terms in the a equation are primarily associated with the decay of a. We present an algebraic

closure approximation for a that results in a heat flux that is the sum of contributions due to gradient and directed transport. Our a-equation is compared with similar equations in the literature.

B. The Equations of a Low Mach Number Flow with Large Density Variations

For the low Mach number flow of a single component ideal gas with large density variations, the equations are the following:[19]

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 , \qquad \textit{(continuity)} \tag{1}$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) + \nabla p = \nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{g} , \qquad \textit{(momentum)} \tag{2}$$

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho \mathbf{u} h) = \frac{dP}{dt} + Q , \qquad \textit{(enthalpy)} \tag{3}$$

$$\mathbf{P}(t) M_\omega = \rho R T , \qquad \textit{(thermal equation of state)} \tag{4}$$

and

$$h(T) = \int^{T} c_p(t)\, dt , \qquad \textit{(caloric equation of state)} \tag{5}$$

where σ is the laminar viscous stress tensor, Q is the volumetric rate of heating due to such sources as chemical reaction or divergence of the laminar heat flux, $\mathbf{P}(t)$ is the volume average pressure of the system, $p(\mathbf{x},t)$ is the pressure fluctuation from the mean value $\mathbf{P}(t)$, and M_ω is the molecular weight of the gas. For low Mach number flows $|p|/\mathbf{P} \approx M^2$, where M is the Mach number.[17] From these equations one can derive an equation for the divergence of the velocity field:[19]

$$\nabla \cdot \mathbf{u} = -\frac{1}{\gamma \mathbf{P}} \frac{d\mathbf{P}}{dt} + \frac{\gamma - 1}{\gamma \mathbf{P}} Q \tag{6}$$

In an open flow system, $\mathbf{P}$ is just the ambient pressure; for flow in a closed volume V, an equation for P can be derived by integrating (6) over V:

$$\frac{1}{\gamma \mathbf{P}} \frac{d\mathbf{P}}{dt} = -\frac{1}{V} \frac{dV}{dt} + \frac{\gamma - 1}{\gamma \mathbf{P}} \frac{1}{V} \int_V Q\, dv \tag{7}$$

C. The Averaged Equations

In our turbulence equations we will use both unweighted averaged quantities and Favre (density-weighted) averaged quantities. The unweighted average and Favre average of a quantity ϕ are defined respectively by

$$\bar{\phi}(\mathbf{x}, t) = \frac{1}{NE} \sum_a \phi_a(\mathbf{x}, t) \tag{8}$$

and

$$\tilde{\phi}(\mathbf{x}, t) = \frac{1}{\bar{\rho}(\mathbf{x}, t)} \frac{1}{NE} \sum_{a} \rho_a(\mathbf{x}, t) \phi_a(\mathbf{x}, t) \tag{9}$$

where ensemble averages are used, ϕ_a being the value of ϕ in a particular experiment a and NE being the number of experiments in the ensemble. The fluctuations from these averages are denoted by

$$\phi' = \phi_a - \bar{\phi} \tag{10}$$

and

$$\phi'' = \phi_a - \tilde{\phi} , \tag{11}$$

where we drop the subscript a on the fluctuations.

By averaging Eqs. (1)-(5) we obtain the turbulence equations:

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{\mathbf{u}}) = 0 , \tag{12}$$

$$\frac{\partial \bar{\rho} \tilde{\mathbf{u}}}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{\mathbf{u}} \tilde{\mathbf{u}}) + \nabla \bar{p} = \nabla \cdot \mathbf{R} + \nabla \cdot \bar{\boldsymbol{\sigma}} + \bar{\rho} \mathbf{g} , \tag{13}$$

$$\frac{\partial \bar{\rho} \tilde{h}}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{h} \tilde{\mathbf{u}}) = \frac{d \bar{P}}{dt} + \bar{Q} - \nabla \cdot \boldsymbol{\phi}^h , \tag{14}$$

$$\bar{P} M_w = \bar{\rho} R \tilde{T} , \tag{15}$$

and

$$\tilde{h} = \int_{T_0}^{\tilde{T}} c_p(t) dt , \tag{16}$$

where the Reynolds stress $\mathbf{R}$ is given by $-\overline{\rho \mathbf{u}'' \mathbf{u}''}$ and the turbulent heat flux $\boldsymbol{\phi}^h$ is given by $\overline{\rho \mathbf{u}'' h''}$. In deriving Eq. (16) we have assumed that the characteristic temperatures over which significant changes in c_p occur, are much larger than characteristic temperature fluctuations T''.

D. An Alternative Expression for $\boldsymbol{\phi}^h$

An alternative expression for the turbulent heat flux can be derived from the averaged and unaveraged equations of state. Subtracting (15) from (4) results in

$$P' M_w = \rho R T - \bar{\rho} R \tilde{T} = \rho R T'' + \rho' R \tilde{T} \tag{17}$$

We now assume that

$$|P'| \ll \bar{P} \quad \text{and} \quad |\rho'| \ll \bar{\rho} \tag{18}$$

Under this assumption the left-hand side of (17) can be neglected, and we obtain

$$\tilde{T}'' = -T\frac{\rho'}{\rho}, \tag{19}$$

wherein temperature and density fluctuations are directly related.

The assumption (18) requires some discussion. It will certainly be true for an open flow system, because the P is always the ambient pressure and never fluctuates. In a closed system, such as in internal combustion engine cylinder, there can be significant fluctuations in the mean pressure P, primarily due to fluctuations in the chemical heat release rate. In an internal combustion engine these are referred to as cycle-to-cycle variations, and there is currently some debate[20] whether or not these cycle-to-cycle variations should be called turbulence. We recommend that in performing the averages (8) and (9) one should use only experiments for which the mean pressure history $P(t)$ is nearly equal to $\bar{P}(t)$. When this limited ensemble average is used, the assumption (18) is automatically satisfied.

Subtracting (16) from (5) gives

$$h'' = \int_{\tilde{T}}^{\tilde{T}+T''} c_p(t)\,dt = c_p(\tilde{T})\,T'', \tag{20}$$

where again we use the assumption that c_p varies little for temperature changes equal to T''. Using (20) and (19) in the defining formula for ϕ^h gives

$$\begin{aligned}\phi^h &= \overline{\rho u'' h''} \\ &= -c_p(\tilde{T})\,\tilde{T}\,\overline{\rho' u''} \\ &= \bar{\rho}\,c_p(\tilde{T})\,\tilde{T}\,\mathbf{a}\end{aligned} \tag{21}$$

where

$$\mathbf{a} = \widetilde{\mathbf{u}''} = \bar{\mathbf{u}} - \tilde{\mathbf{u}}. \tag{22}$$

Equation (21) is the alternative expression we seek for the heat flux. It says that ϕ^h is proportional to a quantity a that can be loosely thought of as the difference between the volume-averaged and mass-averaged velocities. In a two-density or two-phase system, a is proportional to the difference between the velocities of the two phases. In order to investigate further the nature of the turbulent heat flux, we must derive a transport equation for a.

E. The Transport Equation for a

The transport equation for a is obtained by subtracting the equation for the mass-averaged velocity $\tilde{u}$ from that for the volume-averaged velocity $\bar{u}$. The result is

$$\frac{\partial \mathbf{a}}{\partial t} + \overline{\mathbf{u}\cdot\nabla\mathbf{u}} - \tilde{\mathbf{u}}\cdot\nabla\tilde{\mathbf{u}} + \left(\frac{\overline{1}}{\rho} - \frac{1}{\overline{\rho}}\right)\nabla\bar{p} + \overline{\frac{1}{\rho}\nabla p'}$$

$$= -\frac{1}{\overline{\rho}}\nabla\cdot\mathbf{R} + \left(\frac{\overline{1}}{\rho} - \frac{1}{\overline{\rho}}\right)\nabla\cdot\bar{\sigma} + \overline{\frac{1}{\rho}\nabla\cdot\sigma'} \tag{23}$$

As an aid in modeling some of the terms in Eq. (23) we will derive an a-equation for two-phase flows and compare this with Eq. (23). It will turn out that all of the terms in Eq. (23), with the exception of those associated with the fluctuating stresses p' and σ', will be duplicated exactly by terms in the a-equation for two-phase flows. The terms $\overline{1/\rho\ \nabla p'}$ and $\overline{1/\rho\ \nabla\cdot\sigma'}$ are then associated with terms in the two-phase a-equation that arise due to momentum exchange between the phases. With this comparison as a guide we postulate a model for the fluctuating stress terms.

We now briefly introduce the equations for two-phase flow. For more details the interested reader should consult Refs. 2 and 3. For simplicity we restrict ourselves to the flow of two incompressible phases. The continuity equations for each phase are

$$\frac{\partial \rho_1 a_1}{\partial t} + \nabla\cdot(\rho_1 a_1 \bar{\mathbf{u}}^1) = J_{21} \tag{24}$$

and

$$\frac{\partial \rho_2 a_2}{\partial t} + \nabla\cdot(\rho_2 a_2 \bar{\mathbf{u}}^2) = J_{12} = -J_{21} \tag{25}$$

In these equations ρ_i are the microscopic (or conditional) densities, which we assume to be constant; $\bar{\mathbf{u}}^i$ are the average velocities within each phase (where the "i" next to the overbar indicates a conditional average in phase i); a_i are the volume fractions of each phase ($a_1 + a_2 = 1$); and J_{21} is the rate of mass transfer per unit volume from phase 2 to phase 1. The momentum equations for each phase are

$$\frac{\partial \rho_1 a_1 \bar{\mathbf{u}}^1}{\partial t} + \nabla\cdot(\rho_1 a_1 \bar{\mathbf{u}}^1\bar{\mathbf{u}}^1) + a_1\nabla\bar{p} = \rho_1 a_1 \mathbf{g} + a_1\nabla\cdot\bar{\sigma} + \nabla\cdot(a_1\mathbf{R}_1) + \mathbf{P}_{21} \tag{26}$$

and

$$\frac{\partial \rho_2 a_2 \bar{\mathbf{u}}^2}{\partial t} + \nabla\cdot(\rho_2 a_2 \bar{\mathbf{u}}^2\bar{\mathbf{u}}^2) + a_2\nabla\bar{p} = \rho_2 a_2 \mathbf{g} + a_2\nabla\cdot\bar{\sigma} + \nabla\cdot(a_2\mathbf{R}_2) - \mathbf{P}_{21} \tag{27}$$

As is commonly done in two-phase flow modeling,[2] we assume here that the phases are in local pressure equilibrium; that is $\bar{p}^1 = \bar{p}^2 = \bar{p}$. The conditional Reynolds stresses $\mathbf{R}_i$ are given by

$$\mathbf{R}_i = -\rho_i \overline{(\mathbf{u} - \bar{\mathbf{u}}^i)(\mathbf{u} - \bar{\mathbf{u}}^i)}^i$$

The rate of momentum exchange per unit volume from phase 2 to phase 1 is denoted by $\mathbf{P}_{21}$.

Average flow variables $\bar{f}$ are related to the averages within each phase $\bar{f}^i$ by

$$\bar{f} = \alpha_1 \bar{f}^1 + \alpha_2 \bar{f}^2 \tag{28}$$

Thus, for example,

$$\bar{\rho} = \alpha_1 \rho_1 + \alpha_2 \rho_2 \tag{29}$$

and

$$\bar{\rho}\tilde{\mathbf{u}} = \alpha_1 \rho_1 \bar{\mathbf{u}}^1 + \alpha_2 \rho_2 \bar{\mathbf{u}}^2$$

By using the relations (29) and adding Eqs. (24) and (25) and Eqs. (26) and (27) we obtain the same total mass and momentum equations, Eqs. (12) and (13), that we have previously derived, when it is realized that

$$\begin{aligned} \mathbf{R} &= \alpha_1 \mathbf{R}_1 + \alpha_2 \mathbf{R}_2 \\ &\quad - \rho_1 \alpha_1 (\bar{\mathbf{u}}^1 - \tilde{\mathbf{u}})(\bar{\mathbf{u}}^1 - \tilde{\mathbf{u}}) \\ &\quad - \rho_2 \alpha_2 (\bar{\mathbf{u}}^2 - \tilde{\mathbf{u}})(\bar{\mathbf{u}}^2 - \tilde{\mathbf{u}}) \end{aligned} \tag{30}$$

Thus the mass-averaged velocity equation is

$$\frac{\partial \mathbf{u}}{\partial t} + \tilde{\mathbf{u}} \cdot \nabla \tilde{\mathbf{u}} + \frac{1}{\rho} \nabla \bar{p} = \frac{1}{\rho} \nabla \cdot \bar{\boldsymbol{\sigma}} + \frac{1}{\rho} \nabla \cdot \mathbf{R} + \mathbf{g} \tag{31}$$

To obtain the a-equation, we will subtract (31) from an equation for $\tilde{\mathbf{u}}$, which will now be derived. By dividing (26) by ρ_1 and (27) by ρ_2 and summing the results, we obtain

$$\begin{aligned} &\frac{\partial \bar{\mathbf{u}}}{\partial t} + \nabla \cdot (\alpha_1 \bar{\mathbf{u}}^1 \bar{\mathbf{u}}^1 + \alpha_2 \bar{\mathbf{u}}^2 \bar{\mathbf{u}}^2) + \left(\frac{\bar{1}}{\rho} \right) \nabla \bar{p} \\ &\quad = \mathbf{g} + \left(\frac{\bar{1}}{\rho} \right) \nabla \cdot \bar{\boldsymbol{\sigma}} + \nabla \cdot \left(\frac{\alpha_1}{\rho_1} \mathbf{R}_1 + \frac{\alpha_2}{\rho_2} \mathbf{R}_2 \right) + \mathbf{P}_{21} \left(\frac{1}{\rho_1} - \frac{1}{\rho_2} \right) \end{aligned} \tag{32}$$

It can be seen that

$$\nabla \cdot \left| a_1 \bar{\mathbf{u}}^1 \bar{\mathbf{u}}^1 + a_2 \bar{\mathbf{u}}^2 \bar{\mathbf{u}}^2 - \frac{a_1}{\rho_1} \mathbf{R}_1 - \frac{a_2}{\rho_2} \mathbf{R}_2 \right| = \nabla \cdot (\overline{\mathbf{u}\mathbf{u}}) = \overline{\mathbf{u} \cdot \nabla \mathbf{u}} + \overline{\mathbf{u} \nabla \cdot \mathbf{u}} \tag{33}$$

Using (33) in (32) and subtracting (31) yields the two-phase a-equation:

$$\frac{\partial \mathbf{a}}{\partial t} + \overline{\mathbf{u} \cdot \nabla \mathbf{u}} - \tilde{\mathbf{u}} \cdot \nabla \tilde{\mathbf{u}} + \overline{\mathbf{u} \nabla \cdot \mathbf{u}} + \left(\frac{\bar{1}}{\rho} - \frac{1}{\bar{\rho}} \right) \nabla \bar{p}$$

$$= - \frac{1}{\bar{\rho}} \nabla \cdot \mathbf{R} + \left(\frac{\bar{1}}{\rho} - \frac{1}{\bar{\rho}} \right) \nabla \cdot \bar{\boldsymbol{\sigma}} + \mathbf{P}_{21} \left(\frac{1}{\rho_1} - \frac{1}{\rho_2} \right) \tag{34}$$

Comparing (34) and (23), we see they agree if

$$\overline{\frac{1}{\rho} \nabla p' - \frac{1}{\rho} \nabla \cdot \boldsymbol{\sigma}'} = \overline{\mathbf{u} \nabla \cdot \mathbf{u}} + \mathbf{P}_{21} \left(\frac{1}{\rho_2} - \frac{1}{\rho_1} \right) \tag{35}$$

This is the relationship we seek between the fluctuating stress terms and the two-phase momentum transfer terms. To obtain closure we need to postulate a form for $\mathbf{P}_{21}$, and we will investigate expressions employed in two-phase flow modeling.

F. Expressions for the Momentum Exchange Rate in Two-Phase Flows

For a dispersed phase 2 of equal-sized spherical particles of radius r in a continuous phase 1, an expression for the momentum transfer term is[21]

$$\mathbf{P}_{21} = \frac{3}{8} c_D \frac{\rho_1 a_2}{r} |\bar{\mathbf{u}}^2 - \bar{\mathbf{u}}^1| (\bar{\mathbf{u}}^2 - \bar{\mathbf{u}}^1) + J_{21} \bar{\mathbf{u}}^2 \tag{36}$$

Thus, $\mathbf{P}_{21}$ has two terms -- one due to aerodynamic drag and one due to mass exchange. This form of the mass exchange term assumes there are no circulation velocities within the particles. Equation (36) has theoretical justification[21] when $\rho_2 >> \rho_1$ and velocities within each phase are sharply peaked near their mean values. It neglects virtual mass effects, Basset history effects, and particle distortions and oscillations.[22]

Motivated by Eq. (36), modelers usually use a similar expression for all two-phase regimes:[2]

$$\mathbf{P}_{21} = K(\bar{\mathbf{u}}^2 - \bar{\mathbf{u}}^1) + J_{21} \bar{\mathbf{u}}^s \tag{37}$$

where K is called the drag function and $\bar{\mathbf{u}}^s$ is some average interface velocity. The quantity K is a positive function of $\rho_1, \rho_2, a_1, a_2, |\bar{\mathbf{u}}^2 - \bar{\mathbf{u}}^1|$, and an entity size r.

If we accept Eq. (37) then one is led to the postulate that the fluctuating stress terms in the a-equation (23) contribute to the decay of $\mathbf{a}$. Indeed one can show that for a two-phase flow

$$\mathbf{a} \quad \frac{a_1 a_2 (\rho_1 - \rho_2)}{\bar{\rho}} (\bar{\mathbf{u}}^2 - \bar{\mathbf{u}}^1), \tag{38}$$

and (38), in conjunction with (35) and (37), gives

$$\overline{\frac{1}{\rho}\nabla p' - \frac{1}{\rho}\nabla\cdot\sigma'} = \overline{\mathbf{u}\nabla\cdot\mathbf{u}} + K'\mathbf{a} + J_{21}\left(\frac{1}{\rho_2} - \frac{1}{\rho_1}\right)\bar{\mathbf{u}}^s , \tag{39}$$

where

$$K' = \frac{\bar{\rho}}{a_1 a_2 \rho_1 \rho_2} K .$$

K' has dimensions of a frequency.

G. Final Form of the a-Equation

After substituting (39) in (23) and some rearrangement of terms one obtains

$$\frac{\partial \mathbf{a}}{\partial t} + \nabla\cdot(\tilde{\mathbf{u}}\mathbf{a} + \mathbf{a}\tilde{\mathbf{u}}) + K'\mathbf{a} + J_{21}\left(\frac{1}{\rho_2} - \frac{1}{\rho_1}\right)\bar{\mathbf{u}}^s + \tilde{\mathbf{u}}\nabla\cdot\tilde{\mathbf{u}} + \frac{b}{\rho}\nabla\bar{p}$$

$$= -\frac{1}{\rho}\nabla\cdot\mathbf{R} - \nabla\cdot(\overline{\mathbf{u}''\mathbf{u}''}) = \frac{1}{\rho}\overline{\mathbf{u}''\mathbf{u}''}\cdot\nabla\bar{\rho} + \frac{1}{\rho}\nabla\cdot(\overline{\rho'\mathbf{u}''\mathbf{u}''}) . \tag{40}$$

Here we have introduced the quantity b as a dimensionless measure of the density fluctuations:

$$b = \bar{\rho}\left(\overline{\frac{1}{\rho}}\right) - 1 \tag{41}$$

If the density fluctuations are not too large, then b is approximately a self-correlation coefficient for density fluctuations:

$$b \approx \frac{\overline{(\rho')^2}}{(\bar{\rho})^2} \tag{42}$$

In fact, Ref. 4 uses

$$B = \overline{(\rho')^2} \tag{43}$$

as a measure of the density fluctuations. We will develop a transport equation for b in future work.

Three further terms in (40) must be modeled. First we deal with the mass exchange term. One can show from (24) and (25) that

$$\nabla\cdot\bar{\mathbf{u}} = J_{21}\left(\frac{1}{\rho_1} - \frac{1}{\rho_2}\right) \tag{44}$$

and hence the fourth and fifth terms on the left-hand side of (40) combine to give

$$\tilde{\mathbf{u}}\nabla\cdot\tilde{\mathbf{u}} + J_{21}\left(\frac{1}{\rho_2} - \frac{1}{\rho_1}\right)\overline{\mathbf{u}}^s = J_{21}\left(\frac{1}{\rho_2} - \frac{1}{\rho_1}\right)(\overline{\mathbf{u}}^s - \tilde{\mathbf{u}}) - \tilde{\mathbf{u}}\nabla\cdot\mathbf{a} \tag{45}$$

We assume that $\tilde{\mathbf{u}}^s = \tilde{\mathbf{u}}$. An assessment of the validity of this assumption must await a precise physical interpretation of the quantity $\tilde{\mathbf{u}}^s$.

Second, for the tensor $\overline{\mathbf{u}''\mathbf{u}''}$ one can show that for two-phase flows

$$\overline{\mathbf{u}''\mathbf{u}''} = -a_1\frac{\mathbf{R}_1}{\rho_1} - a_2\frac{\mathbf{R}_2}{\rho_2} + \left(1 + \frac{(\bar{\rho})^2}{B}\right)\mathbf{aa}\,, \tag{46}$$

where B is defined by (43) and given in two-phase flows by

$$B = a_1 a_2(\rho_1 - \rho_2)^2 \tag{47a}$$

For future reference we also note that

$$b = \frac{B}{\rho_1\rho_2} \tag{47b}$$

in two-phase flows. We define the volume-averaged conditional Reynolds stress $\mathbf{r}$ by

$$\mathbf{r} = a_1\frac{\mathbf{R}_1}{\rho_1} + a_2\frac{\mathbf{R}_2}{\rho_2} \tag{48}$$

As a first approximation, and despite experimental evidence to the contrary in turbulent flame experiments,[9] we assume the conditional Reynolds stresses are equal and isotropic. Then

$$\frac{\mathbf{R}_1}{\rho_1} = \frac{\mathbf{R}_2}{\rho_2} = \mathbf{r} = -\frac{2}{3}k'\mathbf{I} \tag{49}$$

where k' is related to the specific turbulent kinetic energy $k = \frac{1}{2}(\mathbf{u}'')^2$ by

$$k = k' + \frac{1}{2}\frac{\mathbf{a}^2}{b} \tag{50}$$

A transport equation for k will be developed in future work.

We also use a two-density distribution to model the triple correlation term in Eq. (40). After some algebraic manipulation and use of the assumption (49) one obtains

$$\rho\overline{\mathbf{u}''\mathbf{u}''} = \bar{\rho}\left(1 - \frac{1}{b} + \frac{\bar{\rho}^2}{B}\right)\mathbf{aa} \tag{51}$$

By substituting (45), (46), (49), and (51) in (40) and using the approximation (42) we obtain the final form of the **a**-equation:

$$\frac{\partial \mathbf{a}}{\partial t} + \tilde{\mathbf{u}} \cdot \nabla \mathbf{a} + \mathbf{a} \nabla \cdot \tilde{\mathbf{u}} + \mathbf{a} \cdot \nabla \tilde{\mathbf{u}} + \nabla \cdot (\mathbf{a}\mathbf{a}) + \frac{b}{\bar{\rho}} \nabla \bar{p}$$

$$= -K' \mathbf{a} + \frac{\mathbf{a}\mathbf{a}}{b} \cdot \frac{\nabla \bar{\rho}}{\bar{\rho}} + \frac{2}{3} \left(k - \frac{1}{2} \frac{\mathbf{a}^2}{b} \right) \frac{\nabla \bar{\rho}}{\bar{\rho}} \tag{52}$$

H. An Algebraic Closure Approximation

In numerical computations of multidimensional fluid flows, use of Eq. (52) would require solving two or three additional transport equations for components of **a**. Although this is not an unrealistic task for modern computers, considerable computational efficiency would result if an accurate algebraic closure approximation for **a** could be found. In this section we present such an approximation based on an assumption whose validity must be tested in experimental comparisons. The resulting expression for **a** predicts gradient heat transport, but also contains a contribution that predicts the directed flux arising from the interaction of pressure gradients and density inhomogeneities.

The assumption we make is analogous to the drift flux approximation of two-phase flow modeling.[2] In two-phase modeling this assumption is that the two velocity fields are so tightly coupled through the drag terms that characteristic drag times are much smaller than characteristic flow times. For us the assumption is that

$$K' >> \frac{u_0}{L}, \tag{53}$$

where u_0 and L are a characteristic velocity and gradient length for the flow.

Assuming (53) is true, order of magnitude estimates of the terms in (52) show all terms on the left-hand side can be neglected, except the pressure gradient term. On the right-hand side, the dyadic product term **aa** is negligible since Eqs. (38) and (47) show that **a**/b is proportional to the velocity difference between fluid elements of different density. The resulting equation for **a** becomes

$$\mathbf{a} = \frac{1}{K'} \left| -\frac{b}{\bar{\rho}} \nabla \bar{p} + \frac{2}{3} k \cdot \frac{\nabla \bar{\rho}}{\bar{\rho}} \right| \tag{54}$$

Equation (54) can be put in a more recognizable form if we use

$$\frac{\nabla \bar{\rho}}{\bar{\rho}} = -\frac{\nabla \tilde{T}}{\tilde{T}}$$

$$\mathbf{a} = \frac{1}{K'} \left| -\frac{b}{\bar{\rho}} \nabla \bar{p} - \frac{2}{3} k \frac{\nabla \tilde{T}}{\tilde{T}} \right| \tag{55}$$

In conjunction with (21), Eq. (55) gives a heat flux that is the sum of contributions proportional to $-\nabla \bar{p}$ and $-\nabla \tilde{T}$. The former is the directed flux. It goes to zero in the absence of density fluctuations b

The gradient transport term in (55) looks similar to the gradient heat flux commonly used in turbulence modeling, but there is a difference. The usual form used for the turbulent heat flux[8] is

$$\boldsymbol{\Phi}^h = -\bar{\rho} c_p \frac{\tilde{k}^2}{Pr_T \tilde{\varepsilon}} \nabla \tilde{T} \tag{56}$$

where Pr_T is the turbulent Prandtl number and $\tilde{\varepsilon}$ the turbulence dissipation rate. Equation (56) agrees with the heat flux contribution obtained from the second term in (55) if the drag time associated with fluid elements of differing density equals the turbulence dissipation time. For the momentum exchange function (36) it can be seen that the drag time is

$$\frac{1}{K'} \approx \frac{\rho_2}{\rho_1} \frac{r}{|\bar{\mathbf{u}}^1 - \bar{\mathbf{u}}^2|} \tag{57}$$

when ρ is approximately unity. On the other hand, the turbulence dissipation time is

$$\frac{\tilde{k}}{\tilde{\varepsilon}} \approx \frac{L}{\tilde{k}^{\frac{1}{2}}}, \tag{58}$$

where L is a turbulence length scale. Equations (57) and (58) agree if $r \approx L$, $\tilde{k}^{\frac{1}{2}} \approx |\bar{\mathbf{u}}^1 - \bar{\mathbf{u}}^2|$ and $\rho_1 \approx \rho_2$, but when these equalities are violated more accurate heat fluxes could be obtained using a drag time, and not a turbulence dissipation time, to evaluate the heat flux vector.

III. COMPARISON WITH OTHER WORK

In this section we compare our **a**-equation with two others in the literature. In the BML formulation for turbulent flames,[10] an equation is kept for the turbulent flux of reaction progress variable c. Our quantity **a** is just a constant times the turbulent flux of c:

$$\overline{\rho u'' c''} = \frac{\rho_r \rho_p}{\rho_r - \rho_p} \mathbf{a}, \tag{59}$$

where ρ_r and ρ_p are the reactant and product densities. Two differences are observed between the **a**-equation one derives from the BML formulation and ours. First, in the BML formulation it is not assumed that the conditional Reynolds stresses within each phase are equal and isotropic. An equation for the unconditional Reynolds stress **R** is retained, and the difference between the conditional Reynolds stresses is modeled using **R**. Accordingly, the double and triple correlation terms on the right-hand side of (40) are modeled in a more detailed fashion, although the authors observe[10] that "this modeling is generally not found to be too critical to the predictions of first- and second-moment unconditional quantities."

The second difference is in the modeling of the fluctuating stress terms. The authors follow Launder[23] and model

$$\overline{\frac{1}{\rho}\frac{\partial p'}{\partial x}} = 2c_{1_c}\frac{\tilde{\varepsilon}}{\tilde{k}}\mathbf{a} - c_{2_c}\mathbf{a}\cdot\nabla\mathbf{u} \tag{60}$$

where c_{1_c} and c_{2_c} are empirical constants. Comparison with Eq. (39) shows that these models have in common the decay of a term and that these would be the same if

$$K' = 2c_{1_c}\frac{\tilde{\varepsilon}}{\tilde{k}} . \tag{61}$$

Besnard, Harlow, and Rauenzahn[4] keep equations for both the turbulent heat flux and the quantity $\mathbf{A} = \overline{\rho' \mathbf{u}'}$, which is related to a by

$$\mathbf{A} = -\bar{\rho}\,\mathbf{a} , \tag{62}$$

since they are interested in more complicated equations of state in which the relation (19) does not hold. Their a-equation differs from ours in several respects. An equation for the Reynolds stress is retained and used in modeling the first term on the right-hand side of (40). The triple correlation is broken into two terms

$$\overline{\rho'\mathbf{u}''\mathbf{u}''} = -2\bar{\rho}\,\mathbf{a}\mathbf{a} + \overline{\rho'\mathbf{u}'\mathbf{u}'} , \tag{63}$$

and the latter term is modeled by a gradient diffusion of a. There is a decay of a that arises solely from the viscous stress terms.

IV. SUMMARY AND FUTURE WORK

We have derived a transport equation for the quantity a, which is the difference between the volume- and mass-averaged velocities and is simply related to the turbulent heat flux ϕ^h. Using this equation and an assumption analogous to the drift flux approximation of two-phase flow modeling, we have obtained an algebraic closure relation for ϕ^h that exhibits fluxes due to directed transport proportional to $-\nabla\bar{p}$ and due to gradient transport proportional to $-\nabla T$.

Much work remains to be done before the model can be used in predictive calculations of low Mach number flows with large density variations. The equation for a involves an additional scalar b that is a measure of the density fluctuations. An equation for b must be derived and terms in it modeled. We hope to use the a - and b-equations in conjunction with a k - ε turbulence model. The k- and ε-equations must be reexamined to see what modifications are needed when the flows have large density variations. When mass transport is important, such as in many combustion problems, expressions for the turbulent mass flux must be developed.

In an effort to test some of the modeling assumptions we are currently writing a one-dimensional code that solves the turbulence equations of this paper. Computed results will be compared with experimental measurements of Rayleigh-Taylor instability, turbulent premixed flames, and flows with centrifuging and density variations. These results and extensions of the model will be reported in future publications.

ACKNOWLEDGMENTS

The authors gratefully acknowledge many helpful discussions with Drs. Francis H. Harlow, Didier Besnard, and Rick Rauenzahn. This work was supported by the United States Department of Energy, Office of Energy Utilization Research, Energy Conversion and Utilization Technologies Program.

REFERENCES

1. Libby, P. A. and Bray, K. N. C., *AIAA J.* **19**, 205 (1981).

2. Stewart, H. B. and Wendroff, B., *J. Comput. Phys.* **56**, 3, 363 (1984).

3. Anderson, T. B. and Jackson, R., *I and EC Fundamentals* **6**, 4, 527 (1967).

4. Besnard, D., Harlow, F. H., and Rauenzahn, R., "Conservation and Transport Properties of Turbulence with Large Density Variations," Los Alamos National Laboratory report LA-10911-MS (1987).

5. Cook, T. L. and Harlow, F. H., *Int. J. Multiphase Flow* **12**, 1, 35 (1986).

6. Wahiduzzaman, S. and Ferguson, C. R., Eight International Heat Transfer Conference, Paper # 86-IHTC-253, August 1986.

7. Amsden, A. A., et al., "KIVA: A Computer Program for Two- and Three-Dimensional Fluid Flows with Chemical Reactions and Fuel Sprays," Los Alamos National Laboratory report LA-10245-MS (1985).

8. Launder, B. E. and Spalding, D. B., *Computer Methods in Applied Mechanics and Engineering* **3**, 269 (1974).

9. Bray, K. N. C., et al., *Combustion Science and Technology* **25**, 127 (1981).

10. Bray, K. N. C., Libby, P. A., and Moss, J. B., *Combustion and Flame* **61**, 87 (1985).

11. Libby, P. A., *Prog. Energy Combust. Sci.* 11, 83 (1985).

12. Spalding, D. B., Oral presentation to the Conference on Combustion and Nonlinear Phenomena, Les Houches, France (1985).

13. Rivard, W. C., Farmer, O. A., and Butler, T. D., "RICE: A Computer Program for Multicomponent Chemically Reactive Flows at All Speeds," Los Alamos Scientific Laboratory report LA-5812 (1975).

14. Butler, T. D. et al., "CONCHAS: An Arbitrary Lagrangian-Eulerian Computer Code for Multicomponent Chemically Reactive Fluid Flow at All Speeds," Los Alamos Scientific Laboratory report LA-8129-MS (1979).

15. Butler, T. D. et al., *Prog. Energy Combust. Sci.* **7**, 293 (1981).

16. Cloutman, L. D. et al., "CONCHAS-SPRAY: A Computer code for Reactive Flows with Fuel Sprays," Los Alamos National Laboratory report LA-9294-MS (1982).

17. Williams, F. A., *Combustion Theory*, (Benjamin/Cummings Publishing Co., Menlo Park, California, 1985).

18. Bracco, F. V., "Modeling of Two-Phase, Two-Dimensional, Unsteady Combustion in Internal Combustion Engines," Institution of Mechanical Engineers Conference on Stratified Charge Engines, London (1976).

19. O'Rourke, P. J., "The Acoustic Mode in Numerical Calculations of Subsonic Combustion," in *Combustion and Nonlinear Phenomena*, ed. P. Clavin, B. Larrouturou, and P. Pelce (Les Editions de Physique, Les Ulis, France, 1985).

20. Fraser, R. A. and Bracco, F. V., "Cycle-Resolved LDV Integral Length Scale Measurements in an I.C. Engine," SAE paper 880381 (1988).

21. O'Rourke, P.J., "Collective Drop Effects on Vaporizing Liquid Sprays," Los Alamos National Laboratory report LA-9069-T (1981).

22. Clift, R., Grace, J. R., and Weber, M. E., *Bubbles, Drops, and Particles* (Academic Press, New York, 1978).

23. Bradshaw, P. (ed.), *Turbulence*, Topics in Applied Physics Vol. 12 (Springer-Verlag, Berlin, 1976).